A perturbative study of delocalisation transition in one-dimensional models with long-range correlated disorder

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10th June 2002

Abstract

We study the delocalisation transition which takes places in one-dimensional disordered systems when the random potential exhibits specific long-range correlations. We consider the case of weak disorder; using a systematic perturbative approach, we show how the delocalisation transition brings about a change of the scaling law of the inverse localisation length which ceases to be a quadratic function of the disorder strength and assumes a quartic form when the threshold separating the localised phase from the extended one is crossed.

PACS numbers: 73.20.Jc, 72.15.Rn, 72.10.Bg

Recently, one-dimensional (1D) models with correlated disorder have become the object of intense scrutiny, as a consequence of the discovery that specific long-range correlations of the random potential can create a continuum of extended states and give rise to mobility edges [1, 2]. The emergence of a phase of extended states implies that, when the disorder exhibits appropriate long-range spatial correlations, even 1D models can display a metal-insulator transition analogous to the Anderson transition which takes place in three-dimensional disordered systems. Although the results of the works [1, 2] were obtained for discrete lattices, it was soon found that long-range correlations can produce analogous phenomena also in continuous disordered

1

models [3]. The mobility edge predicted in [2] received an experimental confirmation in [4], where the phenomenon was observed in the transmission of microwaves in a single-mode guide with a random array of correlated scatterers. Further progress along this line of research would make possible the realization of 1D devices with specified mobility edges which could be used as window filters in electronic, acoustic or photonic structures, as suggested in [5].

The theoretical and practical importance of the delocalisation transition in 1D models makes desirable to obtain a complete understanding of the role played by correlations in the formation of mobility edges. Unfortunately, the theoretical comprehension of the phenomenon achieved in [2] and in the successive analytical works is not totally satisfactory, because it rests on the assumption of weak disorder and on the use of a second-order approximation scheme. Thus, the delocalisation transition has been defined by the condition that the second-order term of the inverse localisation length (or Lyapunov exponent) vanish over a continuum interval of electronic energies, while higher-order terms of the Lyapunov exponent have been completely neglected. This simplifying approach is effective but incomplete, because it does not clarify the true nature of the "extended" states, leaving open the question of whether they are completely delocalised or not. The aim of this work is to shed light on this point and thus provide a better understanding of the delocalisation transition in 1D models. To this end, we make use of a systematic perturbative approach that allows us to compute the fourth-order term of the Lyapunov exponent. Armed with this result, we are able to ascertain the nature of the extended states and to discuss the differences between Gaussian and non-Gaussian potentials which appear in the localisation properties of 1D models at this refined level of description.

In what follows, we consider the Hamiltonian continuous model defined by the Schrödinger equation

$$- (\hbar^2/2m)\psi''(x) + \varepsilon U(x)\psi(x) = E\psi(x) \tag{1}$$

which describes an electron of energy E moving under the influence of a random potential $U(x)$. We study the case of weak disorder, identified by the condition $\varepsilon \to 0$. To simplify the form of the equations, in the rest of this paper we adopt a system of units such that $\hbar^2/2m = 1$. We consider electrons of positive energy, so that we can write $E = k^2$; since the wavevector k enters model (1) only via the energy, we can restrict our attention to the case $k > 0$ without loss of generality.

We define the statistical properties of the disorder through the moments of the potential $U(x)$. We assume that the model under study is spatially homogeneous in the mean; as a consequence, the n-th moment of the potential

$$\chi_n(x_1, x_2, \ldots, x_{n-1}) = \langle U(x)U(x + x_1) \ldots U(x + x_{n-1}) \rangle$$

depends only on $n-1$ relative coordinates. Here and in the following we use angular brackets $\langle \ldots \rangle$ to denote the average over disorder realizations. We also want the average features of model (1) to be invariant under a change of sign of the potential; therefore we assume that all moments of odd order vanish. Finally, for the sake of mathematical convenience, we temporarily suppose that a correlation length l_c can be defined such that the values $U(x_1)$ and $U(x_2)$ of the potential are statistically independent when the distance between the points x_1 and x_2 is much larger than l_c. To study the case of long-range correlations, we will subsequently relax this hypothesis by taking the limit $l_c \to \infty$.

To determine the average behaviour of the eigenstates of Eq. (1), we introduce the inverse localisation length

$$\lambda(k) = \lim_{x \to \infty} \frac{1}{4x} \ln \langle \psi^2(x)k^2 + \psi'^2(x) \rangle. \tag{2}$$

As a first step to compute the Lyapunov exponent (2), we derive a differential equation for $\psi^2(x)$ and $\psi'^2(x)$. Using Eq. (1) as a starting point, it is easy to show that the vector

$$u(x) = \begin{pmatrix} \psi^2(x) \\ \psi'^2(x)/k^2 \\ \psi(x)\psi'(x)/k \end{pmatrix}$$

obeys the equation

$$\frac{du}{dx} = (\mathbf{A} + \varepsilon\xi(x)\mathbf{B})\, u, \tag{3}$$

where $\xi(x) = U(x)/k^2$ is the scaled potential and the symbols $\mathbf{A}$ and $\mathbf{B}$ stand for the matrices

$$\mathbf{A} = \begin{pmatrix} 0 & 0 & 2k \\ 0 & 0 & -2k \\ -k & k & 0 \end{pmatrix} \quad \text{and} \quad \mathbf{B} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -2k \\ -k & 0 & 0 \end{pmatrix}.$$

At this point our problem consists in extracting information on the average vector $\langle u(x) \rangle$ from the stochastic equation for $u(x)$; this can be done using

3

a method developed by Van Kampen [6], which replaces Eq. (3) with an ordinary differential equation of the form

$$\frac{d\langle u(x)\rangle}{dx} = \mathbf{K}(x)\langle u(x)\rangle. \tag{4}$$

The generator $\mathbf{K}(x)$ in Eq. (4) is a sure operator that can be expressed in terms of a cumulant expansion

$$\mathbf{K}(x) = \sum_{n=0}^{\infty} \varepsilon^n \mathbf{K}_n(x) \tag{5}$$

where the partial generators $\mathbf{K}_n(x)$ are functions of specific combinations (known as "ordered cumulants") of the moments of the random matrix

$$\mathbf{M}(x) = \xi(x) \exp\left(-\mathbf{A}x\right) \mathbf{B} \exp\left(\mathbf{A}x\right). \tag{6}$$

Van Kampen has established a set of systematic rules for constructing all the terms of the series (5); applying his prescriptions one obtains that all generators of odd order are zero because the odd moments of the potential vanish. As for the even-order generators, the zero-th order term has the simple form $\mathbf{K}_0 = \mathbf{A}$, which corresponds to ignoring the random potential. The first term where disorder manifests its effect is the second-order generator

$$\mathbf{K}_2(x) = \int_0^x dx_1 \exp\left(\mathbf{A}x\right) \langle \mathbf{M}(x)\mathbf{M}(x_1)\rangle \exp\left(-\mathbf{A}x\right),$$

which is proportional to the two-point correlator; a refinement of this result is obtained by taking into account the fourth-order term

$$\begin{aligned}
\mathbf{K}_4(x) = \int_0^x dx_1 \int_0^{x_1} dx_2 \int_0^{x_2} dx_3 \exp\left(-\mathbf{A}x\right) \\
\times \left[\langle \mathbf{M}(x)\mathbf{M}(x_1)\mathbf{M}(x_2)\mathbf{M}(x_3)\rangle\right. \\
-\langle \mathbf{M}(x)\mathbf{M}(x_1)\rangle\langle \mathbf{M}(x_2)\mathbf{M}(x_3)\rangle \\
-\langle \mathbf{M}(x)\mathbf{M}(x_2)\rangle\langle \mathbf{M}(x_1)\mathbf{M}(x_3)\rangle \\
\left. -\langle \mathbf{M}(x)\mathbf{M}(x_3)\rangle\langle \mathbf{M}(x_1)\mathbf{M}(x_2)\rangle\right] \exp\left(\mathbf{A}x\right)
\end{aligned}$$

whose integrand constitutes a non-trivial example of ordered cumulant of the matrix (6). Although the rules of Van Kampen make possible to derive every partial generator $\mathbf{K}_n(x)$, for the purpose of this work we can truncate the series (5) and neglect all terms of higher order than the fourth. As can be seen from Eq. (4), the behaviour of $\langle u(x)\rangle$ for $x \to \infty$ is determined by the

4

eigenvalue with the largest real part of the asymptotic generator $\mathbf{K}(\infty) = \lim_{x \to \infty} \mathbf{K}(x)$; we are thus led to the conclusion that, in order to determine the Lyapunov exponent (2) with fourth-order accuracy, we have to solve the secular equation for the truncated asymptotic generator

$$\overline{\mathbf{K}}(\infty) = \mathbf{A} + \varepsilon^2 \mathbf{K}_2(\infty) + \varepsilon^4 \mathbf{K}_4(\infty). \tag{7}$$

Carrying out the calculations, one obtains that the inverse localisation length (2) can be written as

$$\lambda(k) = \varepsilon^2 \lambda_2(k) + \varepsilon^4 \left(\lambda_4^{(G)}(k) + \lambda_4^{(NG)}(k) \right) + o\left(\varepsilon^4\right) \tag{8}$$

where the second-order term has the standard form

$$\lambda_2(k) = \frac{1}{4k^2} \int_0^\infty \chi_2(x) \cos(2kx) dx. \tag{9}$$

As for the fourth-order term of the Lyapunov exponent (8), its first component can be written as

$$\begin{aligned}
\lambda_4^{(G)}(k) &= \frac{1}{16k^5} \varphi_s(k,0) \left[\varphi_c(k,0) + 4\varphi_c(0,0) \right] \\
&\quad - \frac{1}{8k^4} \left[\varphi_c(k,0) + 2\varphi_c(0,0) \right] \int_0^\infty \chi_2(x) x \cos(2kx) dx \\
&\quad + \frac{1}{8k^4} \varphi_s(k,0) \int_0^\infty \chi_2(x) x \sin(2kx) dx \\
&\quad + \frac{1}{4k^4} \int_0^\infty \left[\varphi_c(0,x) \varphi_c(k,x) - \varphi_c^2(0,x) \cos(2kx) \right] dx
\end{aligned} \tag{10}$$

where the functions $\varphi_c(k,x)$ and $\varphi_s(k,x)$ are defined as

$$\begin{aligned}
\varphi_c(k,x) &= \int_x^\infty \chi_2(y) \cos(2ky) dy \\
\varphi_s(k,x) &= \int_x^\infty \chi_2(y) \sin(2ky) dy
\end{aligned} .$$

The second component turns out to be

$$\begin{aligned}
\lambda_4^{(NG)}(k) &= \frac{1}{k^4} \int_0^\infty dx \int_0^x dy \int_x^\infty dz \Delta_4(y,x,z) \\
&\quad \times \left[\cos(2ky) \cos(2kz - 2kx) - \cos(2kz) \right]
\end{aligned} \tag{11}$$

where the symbol $\Delta_4(x_1, x_2, x_3)$ represents the fourth cumulant of the random potential. These formulae show that, in contrast to the relative simplicity of the second-order result (9), the fourth-order terms (10) and (11) exhibit a non-trivial dependence on the binary correlator and on the fourth cumulant, respectively. The greater complexity of the results is a consequence of the more sophisticated description of localisation, which is visualised as

5

an interference effect generated by double scatterings of the electron in the second-order scheme, whereas the fourth-order approximation also takes into account quadruple scattering processes. The more accurate description of the localisation processes makes possible to draw a distinction between Gaussian and non-Gaussian disorders. These two classes of random potentials are necessarily undifferentiated within the framework of the second-order approximation, since the second-order Lyapunov exponent (9) depends only on the second moment of the potential; in the fourth-order description, however, the differences between the two kinds of potentials emerge in the component (11) which, being a function of the cumulant, vanishes if, and only if, the disorder is Gaussian. In conclusion, the separation of the fourth-order term of the Lyapunov exponent in the two components (10) and (11) is justified by the distinct physical character of these two parts: while the former is common to all Gaussian and non-Gaussian potentials with the same two-point correlation function, the latter describes the specific effect of the non-Gaussian nature of the disorder.

To analyse the case of disorder with long-range correlations, we evaluated the form taken by expressions (9) and (10) when the correlation function is

$$\chi_2(x) = \sigma_2 \frac{\sin(2k_c x)}{x} \exp(-x/l_c) \tag{12}$$

and we subsequently took the limit $l_c \rightarrow \infty$, which reduces the correlation function to the form

$$\chi_2(x) = \sigma_2 \frac{\sin(2k_c x)}{x}. \tag{13}$$

This approach is generally successful, but it fails for $k = k_c$ because for this value of the wavevector the asymptotic limit of the generator (5) exists only as long as l_c is finite. Our results for the Lyapunov exponent, therefore, are not valid in a small neighbourhood of k_c.

Inserting the correlation function (12) in Eq. (9) and taking the limit $l_c \rightarrow \infty$, one obtains that the second-order Lyapunov exponent has the form

$$\lambda_2(k) = \begin{cases} \frac{\sigma_2 \pi}{8k^2} & \text{for} \quad 0 < k < k_c \\ 0 & \text{for} \quad k_c < k \end{cases}. \tag{14}$$

Eq. (14) shows that long-range correlations of the form (13) make the second-order Lyapunov exponent vanish when the wavevector k exceeds a critical value k_c. This result was interpreted in [2] as evidence that long-range correlation of the potential can create a continuum of extended states, with a

mobility edge at $k = k_c$. Second-order theory, however, cannot precise the nature of the "extended" states nor define their spatial extension. To overcome this limit, one can compute the fourth-order term (10) of the Lyapunov exponent. Evaluating expression (10) for the correlation function (12) and then taking the limit $l_c \to \infty$, one arrives at the result

$$\lambda_4^{(G)}(k) = \begin{cases} \Lambda_1(k) & \text{for} \quad 0 < k < k_c \\ \Lambda_2(k) & \text{for} \quad k_c < k < 2k_c \\ 0 & \text{for} \quad 2k_c < k \end{cases} \qquad (15)$$

where the functions $\Lambda_1(k)$ and $\Lambda_2(k)$ are defined as

$$\Lambda_1(k) = \frac{\sigma_2^2}{4k^4} \left[\frac{5\pi}{32k} \ln\left(\frac{k+k_c}{k-k_c}\right)^2 - \frac{\pi}{8} \frac{k^2+kk_c+k_c^2}{k_c(k_c^2-k^2)} - I(k) \right]$$

$$\Lambda_2(k) = \frac{\sigma_2^2}{4k^4} \left[\frac{\pi}{8k} \ln\left(\frac{k+k_c}{k-k_c}\right)^2 + \frac{\pi}{8} \frac{2k_c-k}{k_c(k-k_c)} - I(k) \right]$$

with

$$I(k) = \int_0^\infty \mathrm{si}^2(2k_c x) \cos(2kx) dx.$$

The symbol $\mathrm{si}(x)$ in the previous equation represents the sine integral defined as $\mathrm{si}(x) = -\int_x^\infty dt \sin(t)/t$. In Fig. 1 we show the plot of the fourth-order Lyapunov exponent (15) as a function of the wavevector k. As already ob-

Figure 1: Fourth-order term $\lambda_4^{(G)}(k)/\sigma_2^2$ vs. k/k_c
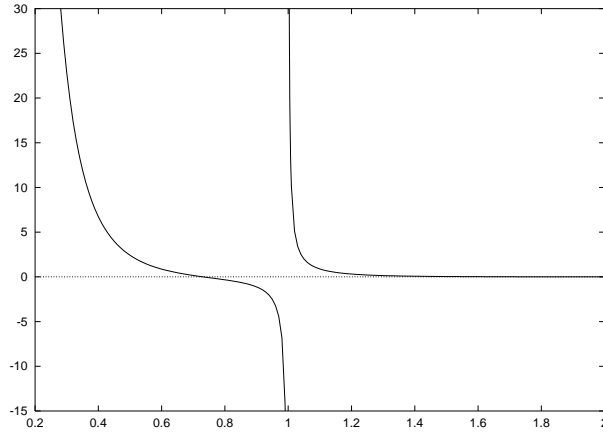
served, the divergence for $k = k_c$ must be disregarded because the asymptotic

7

generator (7) is not defined for this value of the wavevector in the limit of long-range correlations. In the interval $0 < k < k_c$ the second-order Lyapunov exponent (14) is positive and the fourth-order term (15) constitutes just a small correction which enhances or decreases the localisation of electronic states according to whether it assumes positive or negative values. The main interest of Eq. (15), however, lies in the fact that it shows that the fourth-order Lyapunov exponent is positive in the interval $k_c < k < 2k_c$, where the second-order term (14) vanishes. This result clarifies the nature of the mobility edge at $k = k_c$: the electronic states are exponentially localised on both sides of the threshold, but the localisation length is increased by a factor $O(1/\varepsilon^2)$ when the wavevector exceeds the critical value k_c. For weak disorder, the corresponding change in the electron mobility is so conspicuous that one can legitimately speak of "delocalisation transition", even if the "extended" states are not completely delocalised like Bloch states in a crystal lattice. A second noteworthy aspect of the fourth-order term (15) is that it vanishes for $k > 2k_c$ so that, in the case of Gaussian disorder, a second transition takes place at $k = 2k_c$ with the electrons becoming even more delocalised.

So far our discussion has been centred on the term (10), which allows a complete analysis of Gaussian potentials. For non-Gaussian disorder, however, one must also take into account the term (11) which enhances localisation. As an example, one can consider the case of a non-Gaussian potential with long-range binary correlations of the form (13) and with an exponentially decaying fourth cumulant

$$\Delta_4(x, y, z) = \sigma_4 \exp\left[-\beta\left(|x| + |y| + |z|\right)\right]. \tag{16}$$

In this case the fourth-order term of the Lyapunov exponent is the sum of the component (15) and of the additional term

$$\lambda_4^{(NG)}(k) = \frac{15\sigma_4\beta}{8k^2(\beta^2 + k^2)(\beta^2 + 4k^2)(9\beta^2 + 4k^2)} \tag{17}$$

which is obtained by inserting expression (16) in Eq. (10). Since the extra term (17) is always positive, all electronic states with $k > k_c$ are exponentially localised with inverse localisation length proportional to the fourth power of the disorder strength, $\lambda(k) \propto \varepsilon^4$.

The main conclusion of this study is that the delocalisation transition occurring in 1D models with long-range correlated disorder consists in a

change of the scaling behaviour of the Lyapunov exponent when the electronic energy crosses a critical threshold: more specifically, the Lyapunov exponent, which is a *quadratic* function of the disorder strength in the localised phase, assumes a *quartic* form in the extended phase. Another relevant remark is that non-Gaussian potentials produce a stronger localisation effect than their Gaussian counterparts.

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